Supporting Information

Adaptive Accelerated ReaxFF Reactive Dynamics with Validation from Simulating Hydrogen Combustion

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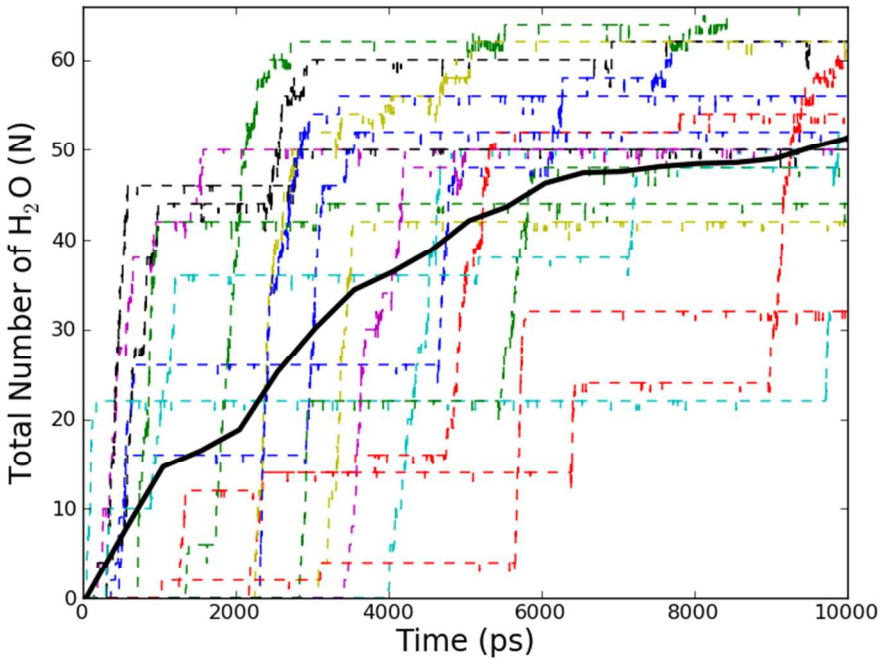

Figure S1. The H2O generation curves of 19 independent BF-RMD simulations at 2498K (slashed lines distinguished by different colors) and the average H2O generation curves of these 19 simulations (black solid line).

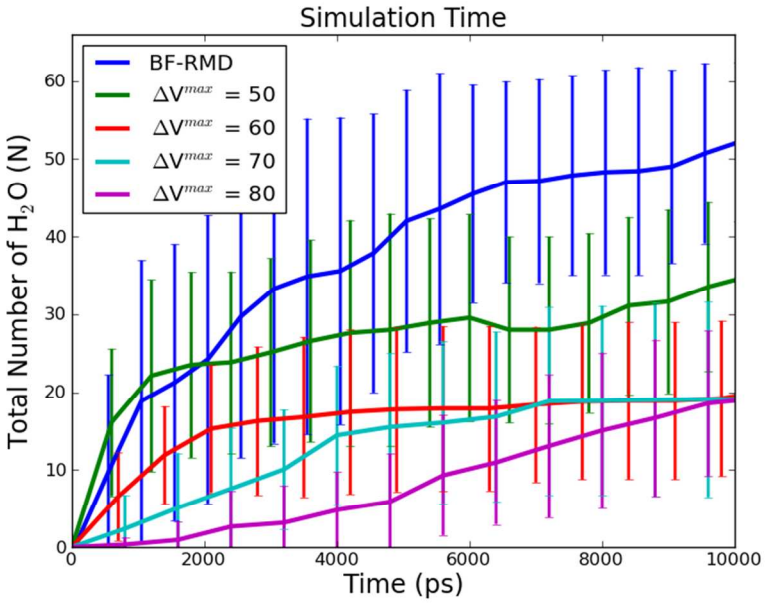

Figure S2. Comparison between BF-RMD and aARRDyn of H2O products generated from combustion of H2 at 2498K as a function of hyper-time. Here we considered ΔV^{max} = 50, 60, 70 and 80 kcal/mol. For BF-RMD, the physical time is the simulation time. For aARRDyn, the physical time is converted to hyper time by reweighing the simulation time using Eqn. 11 as shown in Table 1. The colors are as follows: BF-RMD blue, aARRDyn, with ΔV^{max} =50 kcal/mol green, = 60 kcal/mol red = 70 kcal/mol cyan and = 80 kcal/mol purple. The colors of the error bars are the same as the lines.

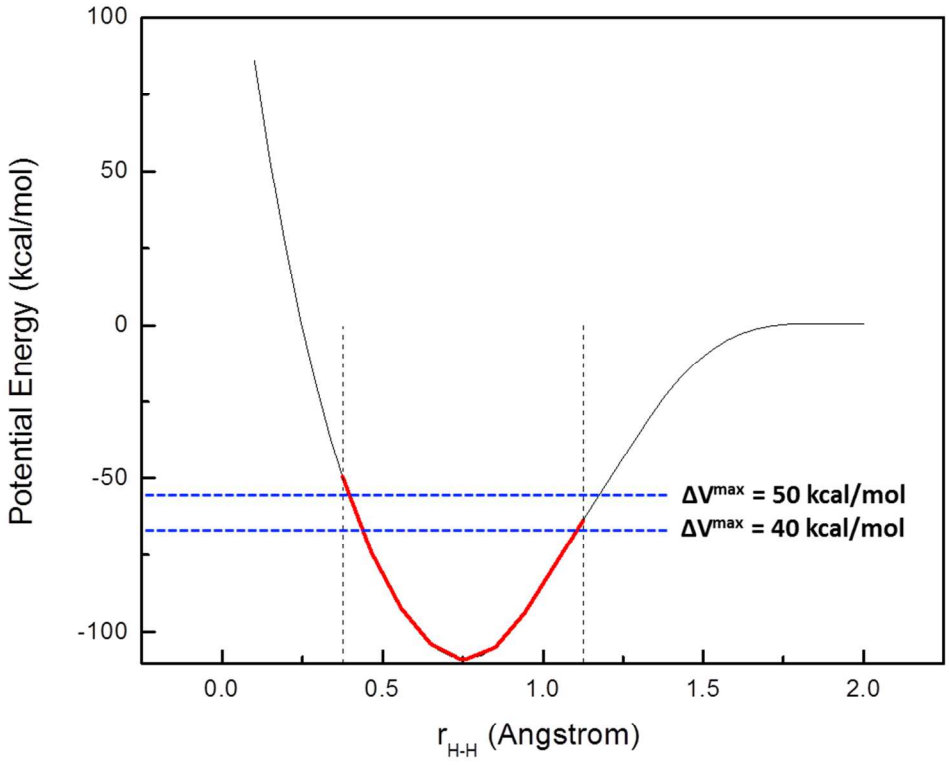

Figure S3. The potential energy as a function of H-H distance (r_{H-H}). Here, the slashed lines label the threshold of boost simulation, 0.375 Å (corresponding to q = -0.5) and 1.125 (corresponding to q = 0.5). The potential energies at these two thresholds are -49.43 kcal/mol and -63.62 kcal/mol. If taking the energy minimum as reference (-108.66 kcal/mol), the relative energies are 59.23 kcal/mol and 45.04 kcal/mol, which may serve as a criteria of the maximum boost potential (ΔV^{max}). Boost potential applied to the red region. The blue square dot shows the ΔV^{max} =40 kcal/mol and ΔV^{max} = 50 kcal/mol. This potential energy curve is derived from an isolated H2 molecular.

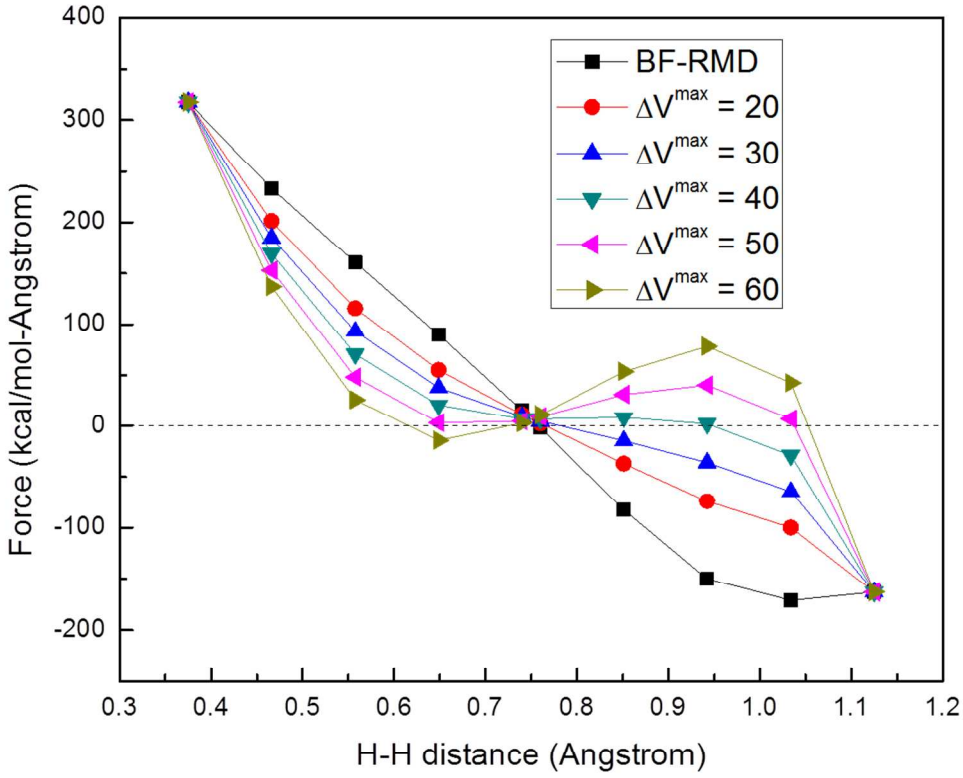

Figure S4. Force between H and H in H_2 at a range of H-H distance (from 0.375 Å to 1.125 Å) at the boost religion as shown in Figure 3. The black line and square symbols stand for brute-force reactive molecular dynamics simulation (BF-RMD). aARRDyn simulations with increasing maximum boost potentials (ΔV^{max}) ranging from 20 kcal/mol to 60 kcal/mol are distinguished by different colors as shown in the legend. The slashed black line shows the zero force for viewing convenience.

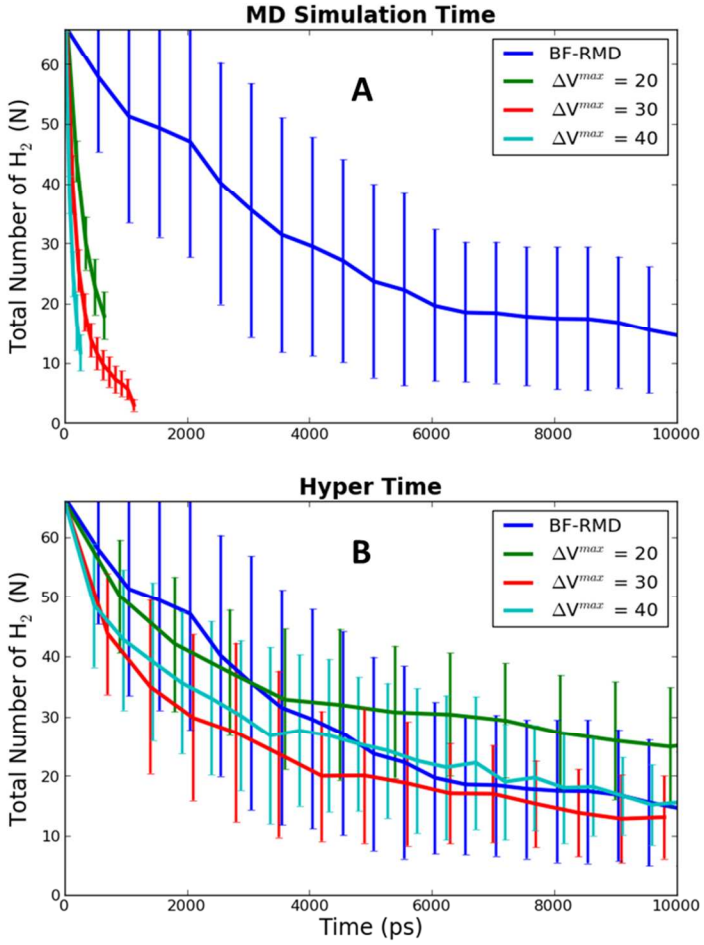

Figure S5. Comparison of H_2 loss as a function of the simulation time (A) and physical time (B) between BF-RMD and aARRDyn with various ΔV^{max} during combustion at 2498K, all using ReaxFF-OH2014. For BF-RMD, the physical time is the simulation time. For aARRDyn, the physical time is hyper time which is converted from reweighing the simulation time. The colors are as following: BF-RMD is in blue. For aARRDyn, the different ΔV^{max} are distinguished in different colors, green, red and cyan, from 20 to 40 kcal/mol. The colors of the error bars are the same as the lines.

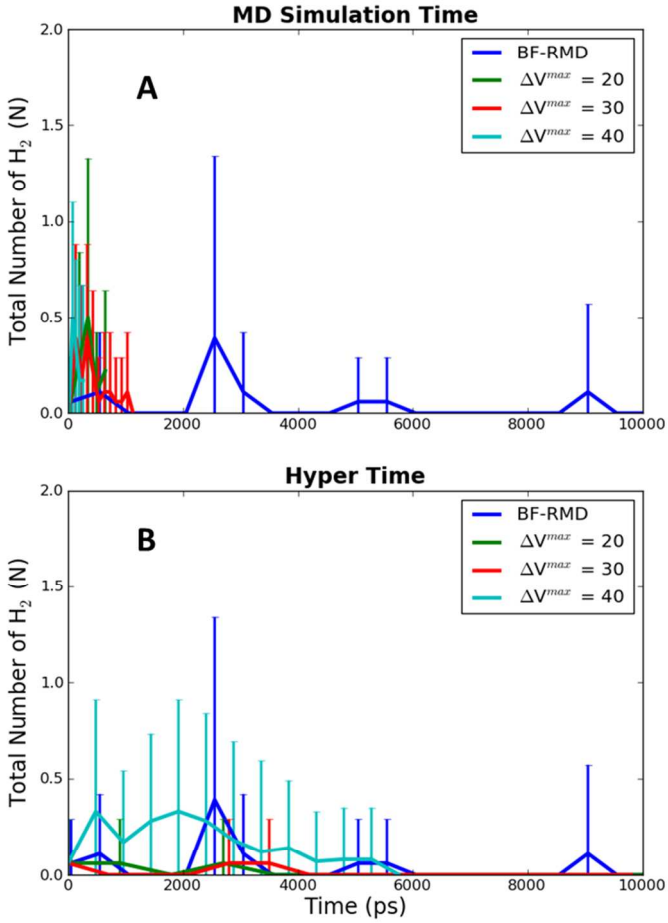

Figure S6. Comparison of H_2O_2 generation as a function of the simulation time (A) and physical time (B) between BF-RMD and aARRDyn with different ΔV^{max} during combustion at 2498K, all using ReaxFF-OH2014. For BF-RMD, the physical time is the simulation time. For aARRDyn, the physical time is hyper time which is converted from reweighing the simulation time. The colors are as following: BF-RMD is in blue. For aARRDyn, the different ΔV^{max} are distinguished in different colors, green, red and cyan, from 20 to 40 kcal/mol. The colors of the error bars are the same as the lines.

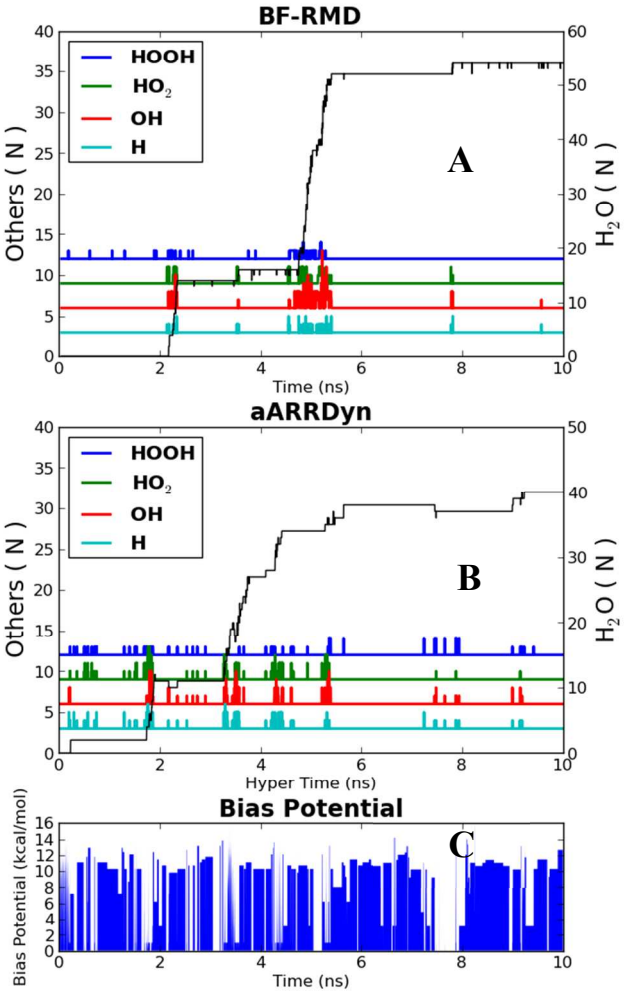

Figure S7. Comparison of the species numbers generated by (A) BF-RMD and (B) aARRDyn simulations (ΔV^{max} = 20 kcal/mol) at 2498 K, all using ReaxFF-OH2014 and (C) the corresponding bias potential. Both simulations were carried out starting from exactly the same initial configuration. The simulation times are 10 ns for BF-RMD and 0.5 ns for aARRDyn. The time shown for aARRDyn is the hyper time from reweighting the simulation time. The populations of H_2O are shown in the right y-axis; the others are shown in the left y-axis. For clarity, the data on H, HO, H_3O, HO_2, and H_2O_2 are shifted by 3, 6, 9, 12, and 15, respectively.

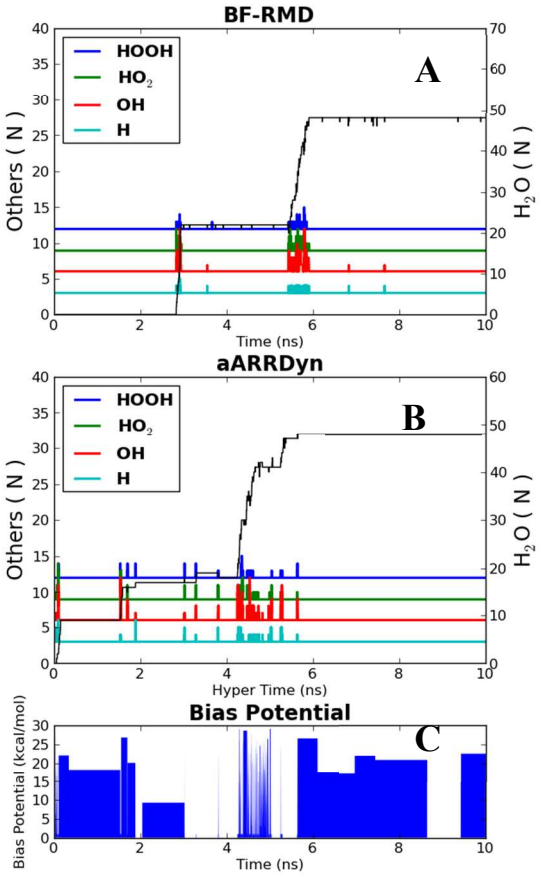

Figure S8. Comparison of the numbers of the species generated by (A) BF-RMD and (B) aARRDyn simulations (ΔV^{max} = 40 kcal/mol) at 2498 K, all using ReaxFF-OH2014 and (C) the corresponding bias potential. Both simulations were carried out starting from exactly the same initial configuration. The simulation times are 10 ns for BF-RMD and 0.5 ns for aARRDyn. The time shown for aARRDyn is the hyper time, from reweighting the simulation time. The populations of H_2O are shown in the right y-axis; the others are shown in the left y-axis. For clarity, the data on H, HO, H_3O, HO_2, and H_2O_2 are shifted by 3, 6, 9, 12, and 15, respectively.

Table S1. Comparison of the dissociation energies between the published ReaxFF-OH2008 force field, the new force field ReaxFF-OH2014 developed herein by fitting to additional QM results. The QM is at the level of B3LYP/6-311G**. The energy unit here is kcal/mol.

Reactions	ReaxFF-OH-2008	ReaxFF-OH-2014	QM
$O_2 = O + O$	-118.74	-125.93	-119.41
$HO_2 = OH + O$	-67.25	-63.21	-65.80
$H_2O_2 = OH + OH$	-43.77	-41.95	-45.69
$H_2 = H + H$	-109.57	-108.72	-106.02
$H_2O = OH + H$	-114.05	-115.35	-112.82
$OH = O + H$	-121.05	-125.97	-100.67
$H_2O_2 = HO_2 + H$	-97.57	-104.72	-80.84
$HO_2 = O_2 + H$	-69.56	-63.25	-47.04
$H_3O = H_2O + h$	-37.34	14.47	15.38

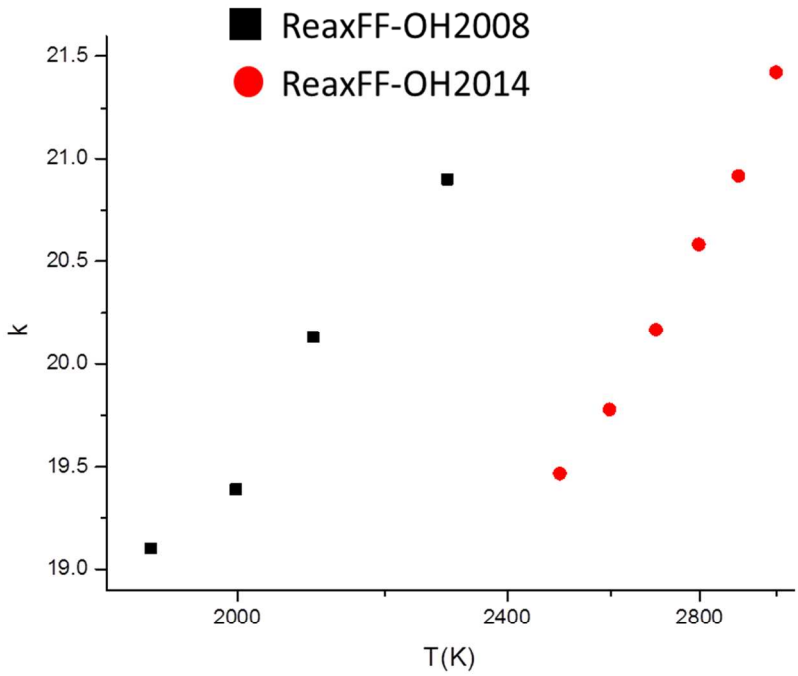

Figure S9. Arrhenius analysis for the overall rate constant of H_2O production derived from BF-RMD NVT simulations at 1898, 1998, 2098 and 2298 K for ReaxFF-OH2008 (black) and simulations at 2498, 2598, 2698, 2798,2898 and 2998 for ReaxFF-OH2014.

Table S2. Comparison of the simulation times (t_{sim}) and hyper times (t_{hyper}) for 50% H2 loss ($t_{reactant}$) and for forming 50% of the H2O products ($t_{production}$) at 1898K all using ReaxFF-OH2008. We consider the BF-RMD simulation along with three cases of aARRDyn, with ΔV^{max} = 20, 30 and 40 kcal/mol. All data in the Table are averaged from 19 independent simulations, with the uncertainties (in parenthesis) estimated from this sampling. The boost factors (the ratio of hyper time and simulation time) are calculated based on $t_{production}$. The excellent agreement of the hyper-time for both loss of reactant and for formation of the validates the aARRDyn methodology

Simulation	ΔV^{max}	$t_{reactant}$ (ns)		$t_{production}$(ns)		Boost factor
		t^{sim}	t^{hyper}	t^{sim}	t^{hyper}	
aARRDyn	40	0.21(0.07)	3.57(4.37)	0.25(0.07)	3.89(4.64)	15.56
aARRDyn	30	0.31(0.11)	3.67(1.24)	0.37(0.10)	3.89(1.51)	10.51
aARRDyn	20	0.72(0.41)	3.52(2.74)	0.81(0.40)	3.68(2.61)	4.54
BF-RMD		3.48(1.79)	3.48(1.79)	3.69(1.67)	3.69(1.67)	1.0

Table S3. Analysis of the reaction frequencies for the final step of H2O production. Listed here are the percentages of those reactions producing more than 1% of the water molecules at 1898 K. The data are obtained from 19 independent simulations by BF-RMD and aARRDyn with ΔV^{max} =20, 30 and 40 kcal/mol. The reactions producing less than 1% are shown in the supporting information (Table S1). The RMS differences are shown in parentheses. The close correspondence between BF-RMD and the three aARRDyn cases validates the aARRDyn methodology, all using ReaxFF-OH2008

	Reactions	aARRDyn (%)			BF-RMD (%)
		40	30	20	
r7	$H_3O + O_2 = H_1O_2 + H_2O$	34(6)	34(7)	34(9)	36(12)
r5	$H_2 + OH = H_1 + H_2O$	25(5)	28(6)	30(7)	30(8)
r8	$HO_2 + H_3O = H_2O + H_2O_2$	8(3)	9(4)	11(4)	11(4)
r4	$H + H_2O_2 = OH + H_2O$	12(3)	11(5)	11(5)	10(6)
r9	$HO_2 + H_3O = H_2O + 2OH$	8(2)	7(3)	5(3)	4(4)
r10	$H_2O_2 + H_3O = OH + 2H_2O$	3(4)	3(3)	2(3)	2(4)
r11	$OH + H_3O = 2H_2O$	4(3)	3(3)	2(3)	1(3)
r12	$HO_2 + H_2O_2 = OH + H_2O + O_2$	1(2)	1(2)	1(2)	1(4)

Table S4. Analysis of the reaction frequencies for H2O2 generation and loss during the simulation. Listed here are the percentages of five major generation reactions (r3, r8, and r13-15) that produce H2O2 molecules and four H2O2 loss reactions (r16, r10, r12, and r14) at 1898 K. The data are obtained from 19 independent simulations by BF-RMD and aARRDyn with ΔV^{max} =20, 30 and 40 kcal/mol. The RMS differences are shown in parentheses. The close correspondence between BF-RMD and the three aARRDyn cases validates the aARRDyn methodology, all using ReaxFF-OH2008

	Reactions	aARRDyn (%)			BF-RMD (%)
		40	30	20	
	H_2O_2 generation				
r3	$H_2 + HO_2 = H + H_2O_2$	37(11)	38(19)	32(12)	36(17)
r8	$HO_2 + H_3O = H_2O + H_2O_2$	38(13)	32(16)	34(16)	29(18)
r13	$2HO_2 = O_2 + H_2O_2$	14(9)	14(8)	18(11)	17(8)
r14	$H + HO_2 = H_2O_2$	11(9)	12(11)	19(8)	13(8)
r15	$H_2O + HO_2 = OH + H_2O_2$	1(13)	5(13)	7(12)	5(14)
	H_2O_2 loss				
r16	$H_2O_2 = 2OH$	50(19)	55(16)	59(17)	52(16)
r10	$H_2O_2 + H_3O = OH + 2H_2O$	21(6)	19(11)	21(11)	17(12)
r12	$HO_2 + H_2O_2 = OH + O_2 + H_2O$	10(6)	8(7)	7(6)	11(10)
r4	$H + H_2O_2 = OH + H_2O$	9(7)	11(9)	10(11)	8(6)

Table S5. Temperature dependence (from 798K to 2998K) of the simulation times (ps) and hyper time (ps) for forming 50% of the H2O products for aARRDyn with ΔV^{max} = 20, 30 and 40 kcal/mol, all using ReaxFF-OH2008. This is compared with the BF-RMD results extrapolated from higher temperature BF-RMD (from Figure 3). All data in this Table are averaged from 19 independent simulations, with the uncertainties quoted in parentheses. The boost factors are calculated based on the ratio of hyper time and simulation time. The RMS differences are shown in parentheses. Note that the BF-RMD* denotes the extrapolated values.

Temperature(K)	ΔV^{max}	H_2O (ps)		Boost factor
		$t^{sim}_{half-life}$	$t^{hyper}_{half-life}$	
798	40	$0.54\times10^{3}(0.06\times10^{3})$	$2.80\times10^{10}(2.30\times10^{10})$	5.18×10^{7}
	BF-RMD*		1.36×10^{10}	
1498	40	$0.35\times10^{3}(0.07\times10^{3})$	$12.21\times10^{4}(6.70\times10^{4})$	348.85
	30	$0.51\times10^{3}(0.13\times10^{3})$	$4.78\times10^{4}(2.40\times10^{4})$	93.72
	20	$1.53\times10^{3}(0.6\times10^{3)}$	$3.81\times10^{4}(2.02\times10^{4})$	24.91
	BF-RMD*		6.91×10^{4}	
1898	40	0.25×10^{3} (0.07×10^{3})	$3.89\times10^{3}(4.64\times10^{3})$	15.56
	30	0.37×10^{3} (0.10×10^{3})	3.89×10^{3} (1.51×10^{3})	10.51
	20	0.81×10^{3} (0.40×10^{3})	3.68×10^{3} (2.61×10^{3})	4.54
	BF-RMD		3.72×10^{3}	
2898	40	64(2)	79(19)	1.23
	30	78(4)	82(9)	1.05
	20	74(8)	76(4)	1.03
	BF-RMD*		66.0	

ReaxFF-OH2014. Reactive MD-force field c/h/o combustion force field: Chenoweth, K.; van Duin, A.C.T.; Goddard, W.A. J. Phys. Chem. A 2008 , 112, 1040-1053. with O-H corrected

39 ! Number of general parameters

50.0000 !p(boc1)

9.5469 !p(boc2)

26.5405 !p(coa2)

1.5105 !p(trip4)

6.6630 !p(trip3)

70.0000 !kc2

1.0588 !p(ovun6)

4.6000 !p(trip2)

12.1176 !p(ovun7)

13.3056 !p(ovun8)

-70.1292 !p(trip1)

0.0000 !Lower Taper-radius (swa)

10.0000 !Upper Taper-radius (swb)

0.0000 !not used

33.8667 !p(val7)

6.0891 !p(lp1)

1.0563 !p(val9)

2.0384 !p(val10)

6.1431 !not used

6.9290 !p(pen2)

0.3989 !p(pen3)

3.9954 !p(pen4)

0.0000 !not used

5.7796 !p(tor2)

10.0000 !p(tor3)

1.9487 !p(tor4)

0.0000 !not used

2.1645 !p(cot2)

1.5591 !p(vdW1)

0.1000 ! (cutoff)

2.1365 !p(coa4)

0.6991 !p(ovun4)

50.0000 !p(ovun3)

1.8512 !p(val8)

0.0000 !not used

0.0000 !not used

0.0000 !not used

0.0000 !not used

2.6962 !p(coa3)

4 ! Nr of atoms; atomID;ro(sigma); Val;atom mass;Rvdw;Dij;gamma;ro(pi);Val(e)
alfa;gamma(w);Val(angle);p(ovun5);n.u.;chiEEM;etaEEM;n.u.
ro(pipi);p(lp2);Heat increment;p(boc4);p(boc3);p(boc5),n.u.;n.u.
p(ovun2);p(val3);n.u.;Val(boc);p(val5);n.u.;n.u.;n.u.

C 1.3825 4.0000 12.0000 1.9133 0.1853 0.9000 1.1359 4.0000
9.7602 2.1346 4.0000 33.2433 79.5548 5.8678 7.0000 0.0000
1.2104 0.0000 199.0303 8.6991 34.7289 13.3894 0.8563 0.0000
-2.8983 2.5000 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000

H 0.7853 1.0000 1.0080 1.5904 0.0419 1.0206 -0.1000 1.0000

9.3557 5.0518 1.0000 0.0000 121.1250 5.3200 7.4366 1.0000

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O 1.2477 2.0000 15.9990 1.9236 0.0904 1.0503 1.0863 6.0000

10.2127 7.7719 4.0000 36.9573 116.0768 8.5000 8.9989 2.0000

0.9088 1.0003 60.8726 20.4140 3.3754 0.2702 0.9745 0.0000

-3.6141 2.7025 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000

X 1.2477 2.0000 15.9990 1.9236 0.0904 1.0503 1.0863 6.0000

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-3.6141 2.7025 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000

6 ! Nr of bonds;

at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(bo5);13corr;n.u.;p(bo6),p(ovun1)

p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)

1 1 156.5953 100.0397 80.0000 -0.8157 -0.4591 1.0000 37.7369 0.4235

0.4527 -0.1000 9.2605 1.0000 -0.0750 6.8316 1.0000 0.0000

1 2 170.2316 0.0000 0.0000 -0.5931 0.0000 1.0000 6.0000 0.7140

5.2267 1.0000 0.0000 1.0000 -0.0500 6.8315 0.0000 0.0000

2 2 156.0973 0.0000 0.0000 -0.1377 0.0000 1.0000 6.0000 0.8240

2.9907 1.0000 0.0000 1.0000 -0.0593 4.8358 0.0000 0.0000

1 3 160.4802 105.1693 23.3059 -0.3873 -0.1613 1.0000 10.8851 1.0000

0.5341 -0.3174 7.0303 1.0000 -0.1463 5.2913 0.0000 0.0000

3 3 60.1463 176.6202 51.1430 -0.2802 -0.1244 1.0000 29.6439 0.9114

0.2441 -0.1239 7.6487 1.0000 -0.1302 6.2919 1.0000 0.0000

2 3 180.4373 0.0000 0.0000 -0.8074 0.0000 1.0000 6.0000 0.5514

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      1.2490    1.0000    0.0000    1.0000   -0.0657    5.0451    0.0000    0.0000
 3      ! Nr of off-diagonal terms. at1;at2;Dij;RvdW;alfa;ro(sigma);ro(pi);ro(pipi)
 1  2    0.1219    1.4000    9.8442    1.1203   -1.0000   -1.0000
 2  3    0.0344    1.6800   10.3247    0.9013   -1.0000   -1.0000
 1  3    0.1131    1.8523    9.8442    1.2775    1.1342    1.0621
18      ! Nr of angles. at1;at2;at3;Thetao,o;p(val1);p(val2);p(coa1);p(val7);p(pen1);p(val4)
 1  1  1  67.2326   22.0695    1.6286    0.0000    1.7959   15.4141    1.8089
 1  1  2  65.2527   14.3185    6.2977    0.0000    0.5645    0.0000    1.1530
 2  1  2  70.0840   25.3540    3.4508    0.0000    0.0050    0.0000    3.0000
 1  2  2   0.0000    0.0000    6.0000    0.0000    0.0000    0.0000    1.0400
 1  2  1   0.0000    3.4110    7.7350    0.0000    0.0000    0.0000    1.0400
 2  2  2   0.0000   27.9213    5.8635    0.0000    0.0000    0.0000    1.0400
 1  1  3  49.5561    7.3771    4.9568    0.0000    0.7533   15.9906    1.0010
 3  1  3  77.1171   39.8746    2.5403  -24.3902    1.7740  -42.9758    2.1240
 2  1  3  65.0000   14.2057    4.8649    0.0000    0.3504    0.0000    1.7185
 1  3  1  74.3994   44.7500    0.7982    0.0000    3.0000    0.0000    1.0528
 1  3  3  77.9854   36.6201    2.0201    0.0000    0.7434   67.0264    3.0000
 3  3  3  80.7324   30.4554    0.9953    0.0000    1.6310   50.0000    1.0783
 1  3  2  71.5018   21.7062    0.4735    0.0000    0.5186    0.0000    1.1793
 2  3  3  84.9468   23.3540    1.5057    0.0000    2.6374    0.0000    1.3023
 2  3  2  77.0645   10.4737    1.2895    0.0000    0.9924    0.0000    1.1043
 1  2  3   0.0000   25.0000    3.0000    0.0000    1.0000    0.0000    1.0400
 3  2  3   0.0000    0.0148    6.0000    0.0000    0.0000    0.0000    1.0400
 2  2  3   0.0000    9.7025    6.0000    0.0000    0.0000    0.0000    1.0400
26      ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n.u;n.u.
 1  1  1  1  -0.2500   11.5822    0.1879   -4.7057   -2.2047    0.0000    0.0000
```

1 1 1 2 -0.2500 31.2596 0.1709 -4.6391 -1.9002 0.0000 0.0000

2 1 1 2 -0.1770 30.0252 0.4340 -5.0019 -2.0697 0.0000 0.0000

1 1 1 3 -0.7098 22.2951 0.0060 -2.5000 -2.1688 0.0000 0.0000

2 1 1 3 -0.3568 22.6472 0.6045 -4.0088 -1.0000 0.0000 0.0000

3 1 1 3 -0.0528 6.8150 0.7498 -5.0913 -1.0000 0.0000 0.0000

1 1 3 1 2.0007 25.5641 -0.0608 -2.6456 -1.1766 0.0000 0.0000

1 1 3 2 -1.1953 42.1545 -1.0000 -8.0821 -1.0000 0.0000 0.0000

2 1 3 1 -0.9284 34.3952 0.7285 -2.5440 -2.4641 0.0000 0.0000

2 1 3 2 -2.5000 79.6980 1.0000 -3.5697 -2.7501 0.0000 0.0000

1 1 3 3 -0.0179 5.0603 -0.1894 -2.5000 -2.0399 0.0000 0.0000

2 1 3 3 -0.5583 80.0000 1.0000 -4.4000 -3.0000 0.0000 0.0000

3 1 3 1 -2.5000 76.0427 -0.0141 -3.7586 -2.9000 0.0000 0.0000

3 1 3 2 0.0345 78.9586 -0.6810 -4.1777 -3.0000 0.0000 0.0000

3 1 3 3 -2.5000 66.3525 0.3986 -3.0293 -3.0000 0.0000 0.0000

1 3 3 1 2.5000 -0.5332 1.0000 -3.5096 -2.9000 0.0000 0.0000

1 3 3 2 -2.5000 3.3219 0.7180 -5.2021 -2.9330 0.0000 0.0000

2 3 3 2 2.2500 -6.2288 1.0000 -2.6189 -1.0000 0.0000 0.0000

1 3 3 3 0.0531 -17.3983 1.0000 -2.5000 -2.1584 0.0000 0.0000

2 3 3 3 0.4723 -12.4144 -1.0000 -2.5000 -1.0000 0.0000 0.0000

3 3 3 3 -2.5000 -25.0000 1.0000 -2.5000 -1.0000 0.0000 0.0000

0 1 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

0 2 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

0 2 3 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000

0 1 1 0 0.0000 50.0000 0.3000 -4.0000 -2.0000 0.0000 0.0000

0 3 3 0 0.5511 25.4150 1.1330 -5.1903 -1.0000 0.0000 0.0000

1 ! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)

3	**2**	**3**	**1.9682**	**-4.4628**	**1.7976**	**3.0000**

Script to plot figure 1

```
import numpy as np
import matplotlib.pyplot as plt

fig = plt.figure()
# sub 2
ax = fig.add_subplot(2,1,2)
bf = np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost13_3_ana/H2O1_b00.dat")
bf = bf.transpose()
a30 =
np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost26_ana/reweight/H2O1_b30.dat")
a30 = a30.transpose()
a40 =
np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost30_ana/reweight/H2O1_b40.dat")
a40 = a40.transpose()
a20 =
np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost34_ana/reweight/H2O1_b20.dat")
a20 = a20.transpose()

ax.errorbar(bf[0][::2000]/4000, bf[1][::2000], bf[4][::2000],
                lw=3, elinewidth=2, label="BF-RMD")
ax.errorbar(a20[0][::600]/4000, a20[1][::600], a20[4][::600],
                lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 20")
ax.errorbar(a30[0][::700]/4000, a30[1][::700], a30[4][::700],
               lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 30")
ax.errorbar(a40[0][::800]/4000, a40[1][::800], a40[4][::800],
```

```
                lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 40")
ax.set_xlim([0,10000])
ax.set_ylim([0,66])
ax.set_xlabel("Time (ps)", size="x-large")
ax.set_ylabel("Total Number of H$_2$O (N)", size="x-large")
ax.set_title("Simulation Time", size="x-large")
ax.legend(loc=4)

# sub1
ax = fig.add_subplot(2,1,1)
bf = np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost13_3_ana/H2O1_b00.dat")
bf = bf.transpose()
a30 = np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost26_ana/H2O1_b30.dat")
a30 = a30.transpose()
a40 = np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost30_ana/H2O1_b40.dat")
a40 = a40.transpose()
a20 = np.loadtxt("/net/hulk/home6/chengtao/PUREMD/bboost34_ana/H2O1_b20.dat")
a20 = a20.transpose()

ax.errorbar(bf[0][::2000]/4000, bf[1][::2000], bf[4][::2000],
                  lw=3, elinewidth=2, label="BF-RMD")
ax.errorbar(a20[0][::400]/4000, a20[1][::400], a20[4][::400],
                  lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 20")
ax.errorbar(a30[0][::400]/4000, a30[1][::400], a30[4][::400],
                lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 30")
ax.errorbar(a40[0][::400]/4000, a40[1][::400], a40[4][::400],
```

```
            lw=3, elinewidth=2, label="$\Delta$V$^{max}$ = 40")
ax.set_xlim([0,10000])
ax.set_ylim([0,66])
ax.set_ylabel("Total Number of H$_2$O (N)", size="x-large")
ax.set_title("Hyper Time", size="x-large")
ax.legend(loc=4)

plt.show()
```

Script to plot figure 2

```
import os
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec



def parse_outcsv(fname, nmax=10000, x=0, y=1, skip=1):
    """
    parse the out.csv
    @param fname: input filename
    @return: list
    """
    data = [[],[]]
    f = open(fname, 'r')
    counter = 0
    for i in f:
        if counter < nmax:
            if counter % skip == 0:
                tokens = [j.strip() for j in i.strip().split(',')]
                if len(tokens) >= y+1:
                    data[0].append(int(tokens[x]))
                    data[1].append(float(tokens[y]))
        counter += 1
    data = np.array(data)
    return data
```

```
def plot_fragments(folder, fragments, labels, ax, maxline=10000, datax=0, datay=1, tag1='',
tag2=''):
    """
    plot the data
    """
    ax1 = ax.twinx()
    counter = 0
    n = 0

    os.chdir(folder)
    for i in fragments:
        data = parse_outcsv('%s.csv'%i, maxline, datax, datay)
        # Plot Data
        if "H2O1" in i:
            ax1.plot(data[0]/4000000.0, data[1], lw=1, color="black")
        else:
            ax.plot(data[0]/4000000.0, data[1]+12-3*counter, lw=2, label=labels[n])
            n += 1
        counter += 1

    xmin = data[0][0]/4000000.0
    xmax = data[0][-1]/4000000.0

    ax.set_xlabel(tag1)
```

```
    ax.set_ylabel(r"Others ( N )", size='x-large')
    ax.set_xlim(xmin,xmax)
    ax.set_xlim(0,10)
    ax.set_ylim(0,40)
    legend = ax.legend(loc=2)
    #ax1.plot([0,20], [66,66], ls='--')
    for label in legend.get_texts():
        label.set_fontweight('bold')

    for label in legend.get_lines():
        label.set_linewidth(2)

    ax1.set_ylabel(r"H$_2$O ( N )", size='x-large')
    ax.set_title(tag2, size="x-large", fontweight='bold')

def plot_bboost(folder, fragments, ax):
    """
    plot the bboost potential
    """
    os.chdir(folder)
    for i in fragments:
        data = np.loadtxt(i)
    ax.fill_between(data[0]/4000000.0, data[1], linewidth=0)
    ax.set_xlim([0,10])
    ax.set_xlabel("Time (ns)")
    ax.set_ylabel("Bias Potential (kcal/mol)")
```

```
    ax.set_title("Bias Potential", size="x-large", fontweight='bold')


def main():
    cwd = os.getcwd()
    # Path for the BF-RMD simulation
    bfrmd = "/net/hulk/home6/chengtao/PUREMD/bboost13_3/"
    # Path for the aARRDyn simulation
    armd = "/net/hulk/home6/chengtao/PUREMD/bboost30/"
    # Fragments to plot
    fragments = [ "H2O2", "H1O2", "H1O1", "H1", "H2O1",]
    labels = ["H$_2$O$_2$", "HO$_2$", "OH", "H", "H$_2$O"]
    # nth sample
    folder = "r17"

    gs = gridspec.GridSpec(5, 5)
    gs.update(hspace=0.55)
    ax1 = plt.subplot(gs[0:2, 0:4])
    ax2 = plt.subplot(gs[2:4, 0:4])
    ax3 = plt.subplot(gs[4, 0:4])

    # Plot the BF-RMD results
    plot_fragments(os.path.join(bfrmd, folder), fragments, labels, ax1, 80000, 0, 1, "Time
(ns)", "BF-RMD")
    # Plot the aARRDyn results
    plot_fragments(os.path.join(armd, folder), fragments, labels, ax2, 80000, 0, 1, "Hyper
Time (ns)", "aARRDyn")
```

```
        # Plot the bboost
        bboost = ['bboost.dat']
        plot_bboost(os.path.join(armd, folder), bboost, ax3)
        os.chdir(cwd)
        plt.show()

if __name__ == "__main__":
        main()
```